201-16554T

IUCLID

Data Set

Existing Chemical	:	ID: 27554-26-3
CAS No.	:	27554-26-3
EINECS Name	:	diisooctyl phthalate
EC No.	:	248-523-5
TSCA Name	:	1,2-Benzenedicarboxylic acid, diisooctyl ester
Molecular Formula	:	C24H38O4
Producer related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	01.11.2000
Substance related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	01.11.2000
Status	:	
Memo	:	ACC Phthalate Esters Panel HPV Testing Group
Printing date	:	05.07.2006
Revision date	:	
Date of last update	:	05.07.2006
Number of pages	:	30
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Contact person	:	Dr. Marian Stanley
Date	:	
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Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers: 68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6 and 111381-90-9 (see remark for names)

Remark : This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers and names:

68515-50-4 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear (DHP)

71888-89-6 1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (DIHP)

27554-26-3 1,2,-benzenedicarboxylic acid, diisooctyl ester (DIOP)

68515-44-6 1,2-benzenedicarboxylic acid, diheptyl ester, branched and linear (DinHP)

111381-89-6 1,2-benzenedicarboxylic acid (C7, C9) ester, branched and linear (79P)

111381-90-9 1,2-benzenedicarboxylic acid, (C7,C11) ester, branched and linear (711P)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower molecular weight transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate subcategories. Of the phthalates in this subcategory, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

03.04.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	-46 °C
Decomposition	:	no, at °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Remark	:	Data are from a peer reviewed literature review of data from a variety of sources including manufacturer's data or handbook values.
Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(2) valid with restrictions This robust summary is assigned a reliability of 2 because there is limited informtion on how the data were developed.
Flag	:	Critical study for SIDS endpoint

05.07.2006 (9)

Value	:	64 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculation
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Melting point calculation by MPBPWIN ver. 1.41 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation. However, the melting point calculation in EPI SuiteTM gives erroneously high results for the phthalate esters.
Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(3) invalid

05.05.2006 (3)

2.2 BOILING POINT

Value	:	417 °C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Boiling point calculation by MPBPWIN ver. 1.41 using calculation method of Stein and Brown.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

05.05.2006 (3)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	.000000252 hPa at 25 °C
Decomposition	:	no
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for vapour pressure, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisooctyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for a diisooctyl phthalate ester was 520.4 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.
Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint
05.05.2006		(1)

Value	:	.00000185 hPa at 25 °C
Decomposition	:	no
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester

Method	:	Vapor pressure calculation by MPBPWIN ver. 1.41 using calculation method of Grain.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

05.05.2006 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	7.73 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for partition coefficient, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisooctyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for a diisooctyl phthalate ester was 520.4 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.
Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.05.2006 (1)

Partition coefficient	:	octanol-water
Log pow	:	8.39 at 25 °C
pH value	:	

Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Partition coefficient by LOGKOWWIN ver. 1.67 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

05.05.2006 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	.00249 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for water solubility, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisooctyl phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for a diisooctyl phthalate ester was 520.4 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths

from 1 to 13 carbons.

Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

05.05.2006 (1)

Solubility in	:	Water
Value	:	.00024 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Water solubility calculated using WSKOWN ver 1.41 based on Kow correlation method of Meylan and Howard. Kow used in calculation was 8.39.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation. EPIWIN is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

05.05.2006 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	1 based on intensity of sunlight
Conc. of substance	:	at 25 °C
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm^3
Rate constant	:	.00000000002056 cm^3/(molecule*sec)
Degradation	:	50 % after 6.2 hour(s)
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson.
Remark	:	50% degradation after 6.24 hrs or 0.52 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration. EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

05.07.2006 (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	3.4 year at 25 °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

12.05.2006 (3)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	390.57
Temperature	25° C
Log Kow	7.73
Water Solubility	0.000249 g/m3
Vapor Pressure	0.0000252 Pa
Melting Point	-46°C

Result : Using the Mackay Level I calculation, the following distribution is predicted for 1,2-benzenedicarboxylic acid, diisooctyl ester:

% Distribution	Compartment
0.0	Air
0.0	Water
97.7	Soil
2.2	Sediment
0.1	Suspended Sediment
0.0	Biota

Test substance : CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
05.05.2006 (6)

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	390.57
Temperature	25° C
Log Kow	7.73

Water Solubility	0.000249 g/m3
Vapor Pressure	0.0000252 Pa
Melting Point	-46°C

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
Air	12.5a
Water	120b
Soil	420c
Sediment	420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI SuiteTM version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on read-across biodegradation data from two phthalate esters: 1,2-benzenedicarboxylic acid, di-C7 alkyl esters (CAS No. 71888-89-6); Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report. 1,2-benzenedicarboxylic acid, diiso-C9 alkyl esters (CAS No. 68515-48-0); Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Result : Using the Mackay Level III calculation, the following distribution is predicted for 1,2-benzenedicarboxylic acid, diisooctyl ester:

Compartment	% Distribution
Air	1.0
Water	8.3
Soil	68.7
Sediment	22.0

Test substance : CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
12.05.2006

(6)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	other: Adapted domestic sewage and soil
Concentration	:	20 mg/l related to Test substance related to
Contact time	:	28 day(s)
Degradation	:	= 57 (±) % after
Result	:	
Deg. product	:	
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Method/Guideline - U.S. EPA 1982, CO2 Evolution, Shake Flask (modified Gledhill). Inoculum - Domestic sewage and soil. Kinetics - Not Reported Degradation Products - Not Reported Analytical Monitoring - Yes
Result	:	Concentration - Nominal test concentration = 20 mg/L for test substance and glucose. Units - % biodegradation Result - >99% primary biodegradation and 57% (s.d. +/-21%) ultimate biodegradation. Primary degradation is expressed as the loss of test substance based on analytical measurements of parent test substance. Ultimate biodegradation is expressed as the percentage of ThCO2 (based on test substance) evolved in each flask.
Test condition	:	Test Conditions - Inoculum was aged for 2 weeks prior to test initiation. The test chemical was added to flasks containing medium and inoculum. The flask were incubated and shaken in the dark for 28 days. Three replicates for CO2 evaluation and 4 replicates for primary degradation were tested. The CO2 production was captured in barium hydroxide solution. Primary biodegradation was determined at the beginning, middle and end by GC FID of entire contents of one replicate. A glucose and blank were also tested. 2 L Erlenmeyer flasks were used as test vessels. The pH at initiation was 7.0 to 7.2. Test flasks were shaken at a rate of 120 rpm at 22 +/- 2 deg C.
Test substance	:	Diisooctyl Phthalate (CAS# 27554-26-3) (1,2,-benzenedicarboxylic acid, diisooctyl ester) Synonym: DIOP No information on purity, but DIOP was analytically confirmed to be within commercial specifications.
Conclusion	:	The substance can biodegrade to a high extent using an acclimated population of microorganisms obtained from a sewage treatment system and soil.
Reliability	:	(1) valid without restriction This summary is rated a "1" because it followed a U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate biodegradation under acclimated conditions, and the results were reviewed for reliability and assessed as valid.
Flag	:	Critical study for SIDS endpoint

12.05.2006 (11) (12)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> .23 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	other
Year	:	1975
GLP	:	yes
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians. Statistical methods-Moving average angle, Probit or Bionomial concentration.
Result	:	96 hr LC50 >0.23 mg/L Mean measured values were used in the LC50 calculation. Nominal test concentrations: control, 0.018, 0.036, 0.072, 0.14, and 0.29 mg/L. Mean measured test concentrations: <0.0040, 0.017, 0.031, 0.060, 0.11, and 0.23 mg/L. Analytical samples were taken at time zero and on a composite of replicates at study termination. Measured values dropped slightly during the exposure period. % Mortality results at 96 hrs per replicate for control and treatment levels: Conc. (mg/L) Rep1/Rep2 Control 0 / 0 0.017 0 / 0 0.031 0 / 0 0.060 0 / 0 0.11 0 / 0 0.23 0 / 0
Test condition	:	Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15L of solution. The diluter maintained a water turnover rate of 5 to 8 tank volumes per day. Two replicates of ten organisms were tested per treatment and control. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection. Fish mean length = 39 mm and mean wet weight = 0.5 g. Test temperature = 12 Deg C. The pH ranged from 7.1 to 7.5. The mean dissolved oxygen ranged from 9.5 to 9.6 mg/L. Ranges of total hardness and alkalinity as CaCO3 of the dilution water were 20 to 26 mg/L and 14 to 22 mg/L, respectively. Fish were obtained from a Montana supplier.
Test substance	:	Diisooctyl Phthalate (CAS# 27554-26-3)

(1,2,-benzenedicarboxylic acid, diisooctyl ester)
Synonym: DIOP
Purity: 100% active ingredient

Conclusion : Test substance is non-toxic to fish at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

08.05.2006 (2) (10)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : > .16 measured/nominal
Analytical monitoring : yes
Method : other
Year : 1975
GLP : yes
Test substance : other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester

Method : Method/Guideline - U.S. EPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975.

Statistical methods - Moving average angle, Probit or Bionomial Concentration.

Result : 48 hr EC50 >0.22 mg/L (based upon time zero analytical samples; no effects at test substance saturation; results from second study). Value was recalculated as >0.16 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997).

Mean measured values were used in the final EC50 calculation.

Nominal test concentrations: control, 0.018, 0.036, 0.072, 0.14, and 0.29 mg/L.
Mean measured test concentrations of time 0 and 48 hr values: <0.0040, 0.017, 0.031, 0.060, 0.11 and 0.23 mg/L.

Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined slightly during study exposure. The high treatment solution is considered the maximum solubility achievable under the conditions of the test.

% Immobility results at 48 hrs per replicate for control and treatment levels in the first test:

Conc. (mg/L)	Rep1/Rep2/Rep3
Control	0 / 0 / 20
0.017	0 / 0 / 40
0.031	20 / 60 / 80
0.060	80 / 80 / 100
0.11	100 / 100 / 100
0.23	100 / 100 / 100

More than 50% of the organisms were trapped on the surface of the 4 higher treatment solutions. Consequently, the study was repeated as a limit

test using a saturated treatment solution.

% Immobility results at 48 hrs per replicate for control and treatment levels in the second limit test:

Conc. (mg/L)	Rep1/Rep2/Rep3
Control	0 / 0 / 0
0.16	0 / 0 / 0

Nominal test concentrations: control and 10 ul/L (saturated solution). Mean measured test concentrations of time 0 and 48 hr values: <0.0037 and 0.16 mg/L. Mean measured values were used in the final EC50 calculation.

Data from the second test are used to characterize the acute toxicity of the test substance.

Test condition : Test treatments were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 30 minutes. The stock solution was prepared at the highest treatment concentration. Dilutions of the stock were prepared for each treatment level. Three replicates of five organisms were tested per treatment. Test vessels were 250 ml beakers with 200 ml of test solution. Analytical method was Gas Liquid Chromatography (GLC).

Water quality parameters for the first test:
Test temperature = 21 Deg C. The pH ranged from 8.3 to 8.5 at initiation and 8.4 to 8.5 on day 2. Dissolved oxygen ranged from 8.5 to 9.0 at initiation and 7.6 to 7.9 on day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

Water quality parameters for the second test:
Test temperature = 20 Deg C. The pH ranged from 7.9 to 8.0 at initiation and 8.4 to 8.5 on day 2. Dissolved oxygen ranged from 8.5 to 9.0 at initiation and was 8.1 in the control and all exposure solution on day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

Test substance : Diisooctyl Phthalate (CAS# 27554-26-3)
(1,2,-benzenedicarboxylic acid, diisooctyl ester)
Synonym: DIOP
Purity: unstated, but believed to be 100% active ingredient because the test material came from the same source as in the rainbow trout acute study.

Conclusion : Test substance is non-toxic to Daphnia at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

08.05.2006 (7) (10)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint :
Exposure period : 6 day(s)
Unit :
EC50 : > 1.3 - measured/nominal
Limit test :
Analytical monitoring : yes

Method	:	other
Year	:	1978
GLP	:	yes
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Method	:	Method/Guideline - EPA 600/9-78-018, Printz Algal Assay Bottle Test. 1978. Statistical methods - Moving average angle, Probit or Bionomial Test type - Static
Result	:	144 hr (6 day) EC50 >2.0 mg/L (based upon time zero analytical samples). Value was recalculated as >1.3 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997). Mean measured values were used in the final EC50 calculation. Nominal test concentration as a percent of a saturated solution: 0 (control) and 100.0%. Mean measured test concentrations of time 0 and 168 hr values: <0.05 and 1.3 mg/L (detection limit was 0.05 mg/L). Analytical samples taken at time zero and on a composite of replicates at termination. In-vivo chlorophyll a, measured until less than 5% change. Both cell number and in-vivo chlorophyll a, measured at termination. Control chlorophyll a or cell counts were not reported. A stimulatory effect of 3 and 19% as compared with the control for chlorophyll a was measured on days 2 and 4, respectively. Analytical samples were taken at time zero and on a composite of replicates at termination. Chlorophyll a percent change relative to control on sampling days and cell number on day 6 results: Conc. Chlorophyll a percent change from control (mg/L) Day 1 Day 2 Day 4 Day 6 Cell # Day 6 1.3 -18 +3 +19 -6 -2
Test condition	:	Algal Growth Medium was used as the control and diluent. 10 uL of test substance was added to 1.0 L of sterile water to form a saturated phthalate solution. This solution was sonicated for 1 minute and allowed to settle for 4 hours. After settling, the water soluble fraction (WSF) was removed for testing. Initial algal concentration was 2.0 E4 cells/ml. Only one treatment level was evaluated (100%WSF) because earlier phthalate testing suggested that toxic effects were not expected with higher molecular weight phthalate esters with low water solubility. Lighting = 4,500 lux, Test temperature = 22+/-2 Deg C. The pH was 7.7 at initiation and ranged from 7.7 to 7.8 on day 6. Algal culture stock was obtained from University of Texas at Austin, TX.
Test substance	:	Diisooctyl Phthalate (CAS# 27554-26-3) (1,2,-benzenedicarboxylic acid, diisooctyl ester) Synonym:DIOP Purity: unstated, but believed to be 100% active ingredient as was provided in the rainbow trout study.
Conclusion	:	Test substance is not toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).
Reliability	:	(2) valid with restrictions Control chlorophyll or cell counts not reported.
Flag	:	Critical study for SIDS endpoint

08.05.2006 (8) (10)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Bacterial
Test concentration	:	10, 100, 1000, and 2000 ug/plate
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1981
GLP	:	no
Test substance	:	other TS: CAS #27554-26-3; 1,2-benzenedicarboxylic acid, diisooctyl ester
Test condition	:	All plates containing >1x108 cells and the test compound were incubated for 40 hours at 370C. The plates were scored for the number of revertants. The results were reported as number of revertants/plate for each indicator strain. To be considered positive, the test results needed to satisfy two criteria: 1) magnitude of the response and 2) dose dependency. The dose dependency criteria was satisfied only if a dose-response effect was evident over three dose levels separated by at least one half log unit. The minimum magnitude of a response needed to be at least twice the response of the vehicle control (DMSO). Positive controls were included for each tester strain. The positive controls for use with metabolic activation included 2-aminofluorene, 2-

aminoanthracene and dimethylbenz(a)anthracene. Positive controls used in the absence of metabolic activation included 2-nitrofluorene, sodium azide and quinacrene mustard.

Test substance	:	1,2,-benzenedicarboxylic acid, diisooctyl ester (diisooctyl phthalate)
Conclusion	:	Under conditions of this study, diisooctyl ester was not mutagenic in the Ames mutation assay.
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

08.05.2006 (4)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	mouse
Sex	:	male/female
Strain	:	CD-1
Route of admin.	:	other: dietary
Exposure period	:	Gestation days 0-17
Frequency of treatm.	:	
Duration of test	:	
Doses	:	0.0, 0.025, 0.05, 0.10, or 0.15% (0, 44, 91, 190.6, or 292.5 mg/kg/bw)
Control group	:	yes
Result	:	NOAEL for maternal toxicity: 0.05% (91 mg/kg); for developmental toxicity: 0.025% (44 mg/kg/day)
Method	:	other: comparable to guideline study
Year	:	1988
GLP	:	no
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, di(2-ethylhexyl) ester (di-ethylhexyl phthalate) 117-81-7
Method	:	Statistical Methods ANOVA; Duncan's Multiple Range Test, Fisher's exact probability test for pairwise comparisons
Result	:	NOAEL NOAEL for maternal toxicity: 0.05% (91 mg/kg). NOAEL for developmental toxicity: 0.025% (44 mg/kg/day). Maternal Effects Actual doses received: 0, 44, 91, 190.6, or 292.5 mg/kg based on body weights and food consumption. No dams died during gestation. Reduced maternal body weight gain was observed in the 0.10 and 0.15% treatment groups. No effects on the number of corpora lutea, implantation sites per dam, the percent pre-implantation loss, and sex ratio of live pups were observed. Embryo/fetal effects The number and percent of resorptions, late fetal deaths, and dead and malformed fetuses were all increased in response to 0.1 and 0.15% treatments. Female fetal weight and the number of live fetuses per litter for both sexes were significantly reduced at 0.10 and 0.15% doses. A

significant increase in both the percentage of fetuses with malformations and the percentage of malformed fetuses per litter were observed with dosing as low as 0.05%. External malformations included unilateral and bilateral open eyes, exophthalmia, exencephaly, and short, constricted, or no tail. Visceral malformations were identified in the major arteries. Noted skeletal defects included fused and branched ribs and misalignment and fused thoracic vertebral centra.

Test condition : After a 7 day quarantine period, breeding pairs were cohabited overnight. Gestation day 0 was determined the morning a vaginal copulation plug was found. Dams were observed daily for signs of clinical toxicity and weights were taken on gestation day 0, 4, 8, 12, 16, and 17. Parameters evaluated following termination included body weight, liver weight, gravid uterine weight, number of ovarian corpora lutea of pregnancy, and status of uterine implantation sites. Fetuses were weighed, examined for external abnormalities and received a visceral examination.

Test substance : 1,2-benzenedicarboxylic acid, di(2-ethylhexyl) ester (di-ethylhexyl phthalate) 117-81-7

Conclusion : Under the conditions of this study DEHP exposure resulted in both maternal and developmental toxicity at high doses.

Reliability : (2) valid with restrictions

08.05.2006 (13)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

Type : other: Reproductive Toxicity
In vitro/in vivo :
Species : mouse
Sex : male/female
Strain : other: Swiss CD-1
Route of admin. : other: dietary
Exposure period : Continuous throughout study (beginning 7 days prior to mating)
Frequency of treatm. : Daily throughout pre-mating, mating, gestation, and lactation
Duration of test : 2 generations
Doses : 0.0, 0.01, 0.10, or 0.3% (~0, 14, 140, or 420 mg/kg)
Control group : other: 40 males and 40 females
Result : NOAEL: 0.01% in the diet (14 mg/kg/day) for fertility and reproductive endpoints
Method : other: no data
Year : 1987
GLP : no data
Test substance : other TS: 1,2-benzenedicarboxylic acid, di(2-ethylhexyl) ester (di-ethylhexyl phthalate) 117-81-7

Method : Statistical Methods
Cochran-Armitage (dose-related trends); Fisher's exact test (mating and fertility trends); Kruskal-Wallis test and Jonckheere's test (group means for sex ratio); Wilcoxon-Mann-Whitney U test (pairwise comparisons of treatment group means).

Result : NOAEL: 0.01% in the diet (14 mg/kg/day) for fertility and reproductive endpoints.

A significant decrease in the number of litters/pair, live pups/litter, mean live pup weight and proportion of live pups was observed at 140 mg/kg/day. Exposure to 420 mg/kg/day resulted in significant infertility during the continuous breeding phase of the study which was seen in both sexes as identified via the crossover mating study. Exposure to the high dose in the crossover study also resulted in male specific effects including reduced testis, epididymis, prostate weights, percentages of motile sperm and abnormal sperm, and sperm concentration in the males. In females effects included reduced combined weight of ovaries, oviducts and uterus. Both

sexes exhibited increased liver weights. The majority of high-dose male mice evidenced some degree of bilateral atrophy of the seminiferous tubules, however; no exposure related histopathology was observed in the females.

Test condition : There were 40 animals/sex in the untreated control group. Males and females in the treatment groups (20 animals/sex) were exposed to the test substance beginning with a 7-day pre-mating period and throughout a cohabitation period for approximately 14 weeks. Reproductive function was assessed during this cohabitation period for number of litters per pair, number of live pups, sex, live births, and pup weight. Following the 14-week cohabitation, the pairs were separated during which any final litters were delivered and kept for assessment of the next generation fertility (F1). Due to an observed effect on fertility, a crossover mating study was performed to determine the affected sex. These mice were evaluated for body weight, organ weights, and sperm indices. When the F1 litters were sexually mature, they were mated with animals from different litters within the same group. The F2 litters were examined for litter size, survival, sex and pup weight. The F1 animals were then necropsied.

Test substance : 1,2-benzenedicarboxylic acid, di(2-ethylhexyl) ester (di-ethylhexyl phthalate) 117-81-7

Conclusion : Under the conditions of this study, DEHP is seen to adversely affect fertility and reproductive performance.

Reliability : (2) valid with restrictions
08.05.2006 (5)

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

05.07.2006

10.3 RISK ASSESSMENT